

Radon Peak-picker

The user manual

Version 1.0

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This manual describes the use of Radon peak-picker GUI based on a neural-network. Symbols used in the manual are explained in the paper ([DOI: 10.1016/j.jmro.2022.100083](https://doi.org/10.1016/j.jmro.2022.100083)).

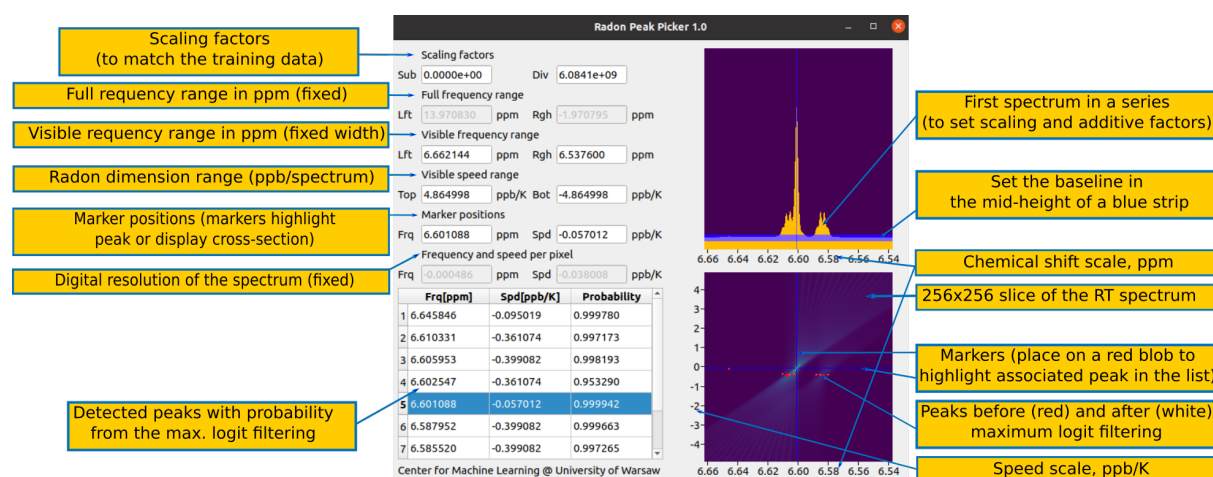


Figure 1: The peak-picker GUI. The right-bottom panel shows the Radon spectrum with detected peaks as white pixels. The right-top panel shows the first Fourier spectrum in the series. The left panel displays settings and a list of detected peaks together with their chemical shifts (ω) and speeds (ϖ).

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| Key | Function | Comment |
|---|--|--|
| ctrl +  /  | Shifting ω by 1 pixel | To change frequency factor |
|  +  /  | Shifting ω by 16 pixels | To change frequency factor |
| ctrl +  /  | Shifting ϖ by 1 pixel | To change speed range |
|  +  /  | Shifting ϖ by 16 pixels | To change speed range |
| ctrl /  +  /  | Change the subtractive factor | Baseline must be at the mid-height of the blue strip |
|  /  | Change in the divisive factor | Peak maximum must not go out of the window |
|  (space) | Transition between the first spectrum in the series and a cross-section through the Radon spectrum | |
|  /  /  /  | Repositioning of markers | |
| Mouse | Function | Comment |
| Left click on the peak table | Move markers to the corresponding white pixel | |

Table 1: List of keyboard and mouse key shortcuts.

System requirements The GUI (`picker.py`) is implemented in Python 3.8 and uses PyQt5 (optionally PyQt6; see the header of the code) for graphical display, so it can be run on any platform and operating system.

Software installation procedure Download the peak-picker package (**picker.zip**) from <http://nmr.cent.uw.edu.pl/downloads/> and unpack it. Inside, there is a `picker.py` and the folder with the neural-network model (folder named **model**).

Manual - the step-by-step procedure (α -asarone example)

1. **Important:** the current version of the program requires the number of time-domain points to be equal to 32768 (after zero-filling) and a number of spectra in a series to be 20. See example data.
2. Process your experimental FIDs (e.g. in TopSpin) by applying phase and baseline correction, possibly also solvent suppression. Do not use zero-filling, apodization other than by exponential function or any other procedures that may cause the peaks to deviate from Lorentzian/Gaussian shape. Save the processed data in an FID format using `ift` and then `genfid` command. **The peak-picker uses ABSF1 and ABSF2 parameters from procs file to set up a frequency (ppm) scale. Please check that these parameters are present and have the correct settings.**
3. Save your data in folders numbered from 1 to 20 in a folder named e.g. **data**.
4. Keep the model folder and the `picker.py` file in the same path.
5. Launch the GUI with a command below specifying the path to the **data** folder, the unit of the parameter varied over the series of spectra (e.g. K) and the difference between its values from spectrum to spectrum (e.g. 1.0):

```
python3 ./picker.py data K 1.0
```

6. The GUI window will appear. The **right-bottom** panel of the GUI will show the 256×256 slice of the Radon spectrum, with a chemical shift scale in ppm and speed scale in ppb/K, generated from the experimental FIDs.

7. Adjust the **speed (ϖ) range** by:
 - (a) changing **one** of the values in the **left panel (Top or Bot)** or
 - (b) moving the spectrum by 1 or 16 pixels by pressing vertical arrows with control or shift, respectively.
8. The visible frequency subrange is displayed in the **the left panel** as chemical shift measured in ppm. To change it:
 - (a) set the displayed chemical shift range by entering **one** of the extreme values (**Lft** or **Rgh**) or
 - (b) move the spectrum by 1 or 16 pixels by pressing horizontal arrows with control or shift, respectively.
9. The **right-top panel** shows the real part of the first Fourier spectrum in the series in the same frequency subrange. In the **lower part**, it displays a horizontal semi-transparent blue strip.
10. Adjust the **subtractive factor (Sub)** so that the baseline is located at the mid-height of this blue strip. This can be done by:
 - (a) editing the subtractive factor in the left panel (**Sub**) or
 - (b) pressing plus or minus with control or shift
11. Then, adjust the **divisive factor (Div)** so that the noise does not protrude the semi-transparent strip and so that all the visible peaks fit within the visible window. This can be done by:
 - (a) editing the divisive factor in the left panel (**Div**) or
 - (b) pressing plus or minus without any modifiers like control or shift
12. The peak-picker predictions are superimposed with the Radon spectrum in the **right-bottom panel**. The pixels classified by the network as peaks are displayed in red. From each red blob separately, the pixel with the maximum logit is selected and displayed in white. The white pixels are the final peak centers predicted by the whole peak-detection pipeline described in the manuscript.
13. The detected peaks are listed in the **left panel**. The table gives their frequencies, ω , in ppm, and the rates of change, ϖ , in ppb/K. The table also lists the probabilities assigned by the network. They are calculated as the sigmoid function of the logits returned by the network, which is standard in binary classification. Probabilities measure the network’s confidence that each white pixel is indeed a peak center.
14. The right panels display a vertical frequency marker visible in both spectra and a horizontal rate-of-change marker visible only in the Radon spectrum. Move the markers by:
 - (a) editing their positions in the left panel or
 - (b) pressing arrows without any modifier keys like control or shift.

When the markers cross within any red blob, the white peak detected in this blob is highlighted in the **left panel**. The markers automatically move to the corresponding white pixel when a peak is mouse-clicked in the left panel. This feature allows identifying the peaks listed to the left in the spectrum displayed to the right and vice versa. You may first move the markers to a red blob in the spectrum and then click the highlighted peak in the table to place the markers exactly at the white pixel in this blob.

The peak-picking errors due to a wrong preprocessing (α -asarone sample) The left panel of the Figure 2 shows the results of peak-picking performed on the data with the significant phase error present in some of the spectra. The wrong phasing leads to false positives in the peak-picking procedure. The right panel shows the result for the correctly phased data.

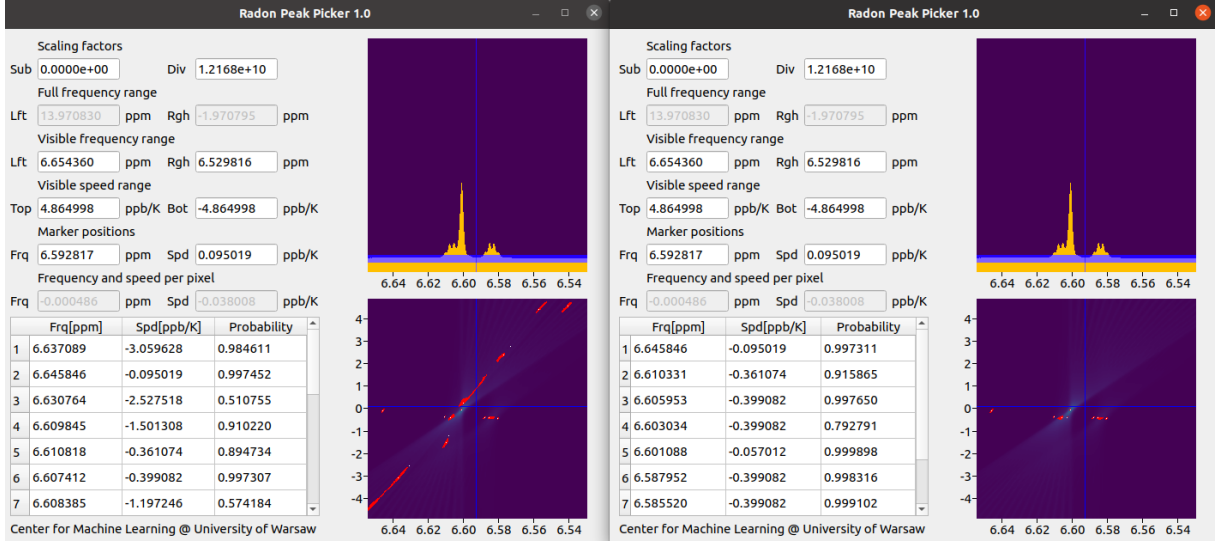


Figure 2: The consequences of improper phasing. The left panel: GUI with the results of peak-picking performed on the wrongly phased data (some of the spectra in a series have major phase errors). The right panel: result for properly phased data.